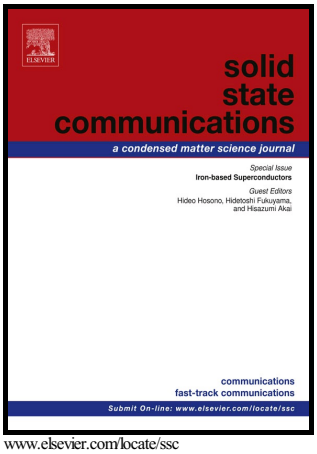

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Hui Zhang, Fan-Sun Meng, Yan-Bin Wu

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Two single-layer porous gallium nitride nanosheets: a first-principles Study

Hui Zhang[a], *Fan-Sun Meng*[b], *Yan-Bin Wu*[a*]
[a]*College of Sciences, Shenyang University, Shenyang 110044, China*
[b]*School of Science, Liaoning University of Technology, Jinzhou 121001, China*
[*]*Corresponding author: yanbinwu@outlook.com*

Abstract

The gallium nitride (GaN) is a novel wide-gap semiconductor for photoelectric devices. In this paper, two 2D single-layer GaN crystal structures, called H-GaN and T-GaN, are discovered by the density functional theory calculations. The phase stability is confirmed by phonon dispersions. The sole-atom-thick crystals of H-GaN and T-GaN, has possess enlarged specific surface area than the graphene-like allotrope (g-GaN) due to the porous structures. In addition, they have indirect band gaps of 1.85~1.89 eV and the electronic structures can be further modulated by applied strains. For example, T-GaN transforms from an indirect semiconductor to a direct one due to compressed strains. Both the combination of high specific surface area and moderate band gaps make these 2D crystals potential high-efficiency photocatalysts. Our results will also stimulate the investigations on 2D GaN nano crystals with rich electronic structures for wide applications.

Keywords: A. Gallium nitride; D. Electronic structure; E. First-principles calculations

1. Introduction

Investigations on the two-dimensional (2D) nanocrystals with atomic-thickness, such as representative graphene, have been the most active field since the discovery of graphene. The single-layer graphene possesses many excellent quantum transport and mechanical properties[1, 2], which is consequently considered one of the most promising materials for future electronics. Nevertheless, the absence of intrinsic band gap, which greatly hampers more wide application of graphene[3], has stimulated exploration of other 2D nanomaterials, such as C_3N_4, phosphorus allotropes and transition metal dichalcogenides (TMDs) [4-9].

Among diverse 2D materials, many 2D BN counterparts have been theoretically explored and experimentally studied.[10, 11] Beyond graphene-like 2D materials, the 2D porous films and nanomaterials[12-15], including porous BN nonosheets [16, 17], have been recently fabricated as high-performance catalysts, due to extremely high specific surface area and special surface activity[18, 19]. However, the 2D forms of AlN and GaN, which belongs to well-known III–V semiconductors for the device applications as well as BN, have seldom been fabricated.[20] Bulk GaN is a wide-gap (~3.5 eV) semiconductor that usually crystallizes in the wurtzite lattice[21]. The graphene-like 2D g-AlN and g-GaN nanosheets have been demonstrated as free-standing[22, 23] due to theoretical calculations. Recently, the synthesis of 2D gallium nitride (GaN) has been reported via a migration-enhanced encapsulated growth (MEEG) technique utilizing epitaxial grapheme.[24] In addition, porous GaN polycrystalline structures have been experimentally formed[25-27]. Based on the previous findings, it is interesting to explore 2D porous GaN crystals with novel electronic strctures.